$YBa_2Cu_4O_8$ KUPRATIDA ZARYAD TASHUVCHISI MASSASI

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Annotatsiya. Ushbu maqolada $YBa_2Cu_4O_8$ kuprati kengaytirilgan Holstein-Hubbard modeli va yuqori T_c o‘tao‘tkazuvchanlikning bipolaron mexanizmi doirasida qaralgan. $YBa_2Cu_4O_8$ kupratida $(3\div4)m_e$ massali yengil (bi)polaronlar mavjudligi ko‘rsatilgan. Polaron massalarining hisoblangan qiymatlari tajriba ma’lumotlarga mos keladi.
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Kalit so‘zlar: kupratlar, $YBa_2Cu_4O_8$, o‘tao‘tkazuvchanlik, Boze-Eynstein kondensatsiyasi, polaron, bipolaron, polaron massasi.

МАССА НОСИТЕЛЯ ЗАРЯДА В КУПРАТЕ $YBa_2Cu_4O_8$

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Аннотация. В статье рассмотрен купрат $YBa_2Cu_4O_8$ в рамках расширенной модели Холстейна-Хаббарда и биполяронного механизма высокотемпературной сверхпроводимости. Показана возможность существования легких (би)поляронов в купрате $YBa_2Cu_4O_8$ с массами $(3\div4)m_e$. Расчетные значения масс поляронов согласуются с экспериментальными данными.
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Ключевые слова: купраты, $YBa_2Cu_4O_8$, сверхпроводимость, Бозе-Эйнштейновская конденсация, полярон, биполярон, масса полярона.

MASS OF CHARGE CARRIER IN $YBa_2Cu_4O_8$ CUPRATE

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Abstract. In this article $YBa_2Cu_4O_8$ cuprate is considered within the framework of extended Holstein-Hubbard model and bipolaronic mechanism of high-T_c superconductivity. A possibility of existence of light (bi)polarons in $YBa_2Cu_4O_8$ cuprate with masses $(3\div4)m_e$ is shown. The calculated values of polaron masses are in agreement with the experimental data.
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Key words: cuprates, $YBa_2Cu_4O_8$, superconductivity, Bose-Einstein condensation, polaron, bipolaron, polaron's mass.

INTRODUCTION

The nature of the high temperature superconductivity (HTSC) of copper oxide materials (cuprates) is still not entirely clear. There are a sufficient number of models claiming the HTSC theory. Each model is required to explain all aspects of the properties of cuprates in the normal and superconducting states. This concerns the transport properties of cuprates in the normal state, in particular the mass of the charge carrier. As it is believed that the path to understanding the mechanism of HTSC in cuprates lies through the understanding of all properties of cuprates in the normal state.

Here, we report on the estimation of the charge carriers' mass in $YBa_2Cu_4O_8$ cuprate within the (bi)polaron point of view. While doing that we rely on the Extended Holstein-Hubbard model (or Fröhlich–Coulomb) [1] and bipolaronic mechanism of HTSC [2] which implies Bose-Einstein condensation (BEC) of a gas or liquid of the intersite bipolarons.

The main idea of our approach was given in the works [3-6]. In the work [3], the values of T_c of $La_{1.85}Sr_{0.15}CuO_4$ and $La_{1.9}Sr_{0.1}CuO_4$ thin films, which were grown on LSAO and STO substrates, were satisfactorily explained. The work [4] extends our approach to $RBa_2Cu_3O_{7-\delta}$ cuprates. The recent works are devoted to the explanation of doping dependencies of T_c of $La_{2-x}Sr_xCuO_4$ thin films [5] and the uniaxial pressure (strain) derivatives of T_c of $La_{2-x}Sr_xCuO_4$ bulk samples [6].

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THEORETICAL MODEL

According to the bipolaron model of superconductivity, HTSC cuprates are due to the BEC of a gas (or liquid) of the intersite bipolarons [2]. Accepting simple assumptions such as: (i) the intersite bipolarons form an ideal gas; (ii) mass of bipolaron is twice of polaron's mass i.e. $m_{bp}=2m_p$ and that the cuprates are (iii) in strong electron-phonon interaction (EPI) limit and (iv) on nonadiabatic regime, one can estimate the BEC, T_{BEC}, of the ideal gas of the intersite bipolarons [3, 4]

$$T_{BEC}=\frac{3.31\hbar^2 n^{2/3}}{2k_B m^{*}}e^{-g^2}, \tag{1}$$

where $\hbar$ (k_B) is Planck's (Boltzmann's) constant, m^{*} is the bare band mass (is set equal to mass of free electron), n is density of the intersite bipolarons and g^2 is the mass renormalization factor of polaronic system. The above reasonings can be justified by the facts that (i) concentration of charge carriers in the cuprates is relatively small (dilute limit); (ii) the Coulomb repulsion between bipolarons is significantly reduced in the cuprate oxides by the ionic screening (page 132 of Ref. [7]). The mass renormalization factor g^2 is defined as [8]

$$g^2=\gamma\frac{E_p}{\hbar\omega}, \tag{2}$$

where

$$\gamma=1-\frac{\sum_m f_m(n)f_m(n+a)}{\sum_m f_m^2(n)} \tag{3}$$

is a numerical coefficient,

$$E_p=\frac{1}{2M\omega^2}\sum_m f_m^2(n) \tag{4}$$

is a polaron shift, M is *apical* oxygen ion's mass and $f_m(n)$ is the *density-displacement* type EPI force defined by analytical formula

$$f_m(n)=\frac{\kappa h_O}{¿¿} \tag{5}$$

Here κ is some coefficient, $¿n-m\vee¿$ is the distance measured in units of the lattice constant a, h_O is Cu(1)-O(2) bond length. For numerical results we rely on the model lattice of chain model of cuprates (Fig. 1) and calculate g^2 for that lattice. The density-displacement type force Eq. (5) was introduced by Alexandrov and Kornilovitch in Ref. [8] in order to mimic an interaction of a hole on CuO_2 plane with the vibrations of *apical* oxygen ions in the cuprates. Convincing evidence for a such coupling of in-plane holes with the c- axis polarized vibrations of apical oxygen ions comes from many experiments (for example [9]). Therefore, here we consider only that component of the electron-lattice force which represents an interaction of a hole on CuO_2 plane with the c- axis polarized apical oxygen vibrations and for the sake of simplicity, we assume that apical oxygen ions are dispersionless Einstein oscillators with the vibration frequency ω. In addition, we estimate the mass renormalization factor g^2 within extended Holstein model (which is consistent with the ideality of Bose gas of intersite bipolarons).

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RESULTS AND DISCUSSION

Now, we apply the above formalism to $YBa_2Cu_4O_8$ cuprate. To do this, consider quasi two-dimensional lattice consisting of CuO_5 pyramids as in $YBa_2Cu_4O_8$. A copper-oxygen (CuO_2) plane of the CuO_5 pyramids we assume as square lattice with the lattice constant a=0.193 nm which mimics planar Cu(2)-O(2) and/or Cu(2)-O(3) distances in $YBa_2Cu_4O_8$ [10]. Cu(2)-O(1) bond length of $YBa_2Cu_4O_8$ which is equal to 0.2276 nm we associate with h_O. All these lattice parameters are measured at 85 K. In addition, for phonon frequency we accept $\hbar\omega$ =75 meV which common for cuprates, and for the mass of apical oxygen we put M=16 a.m.u.. First of all, we choose the value of the polaron energy, E_p =0.75 eV, in such a way that the value of the intersite bipolaron BEC temperature, T_{BEC}, coincides with the experimental value of the critical temperature of superconductivity, T_c=80 K, of $YBa_2Cu_4O_8$. Then, accepting $T_{BEC}=T_c$, we calculate polaron parameters according to the above assumptions and formulas Eq.(1)-Eq.(5). Calculated mass of a polaron corresponding to the chosen polaron energy (shift) E_p=0.75 eV is equal to $m_p=18.3m_e$. The latter mass should be interpreted as three-dimensional mass of polaron in bulk $YBa_2Cu_4O_8$.

Now, we do an estimation of in-plane mass of polaron i.e. mass of polaron within CuO_2-plane, $m_{p,ab}$. In order to calculate in-plane polaron mass $m_{p,ab}$ one uses the following formulas $m_p=m_{p,ab}^{2/3}\cdot m_{p,c}^{1/3}$ and $\gamma_{pm,cab}=m_{p,c}/m_{p,ab}$. The latter coefficient γ_m characterizes anisotropy of transport properties of $YBa_2Cu_4O_8$ along CuO_2-plane and along c-direction. The experimental value of the coefficient $\gamma_{m,cab}$ can be found in works [11-13]. Zech et al., experimentally determined the mass anisotropy ratio $\gamma_{m,cab}=\sqrt{m_c^{¿}/m_{ab}^{¿}}$=12.3 [11]. Using the latter value of the mass anisotropy ratio one easily calculates charge carrier's (polaron's) mass in CuO_2-plane $m_{p,ab}$ =3.489m_e . According to Hussey et al., [12] and Taylor et al., [13] the mass anisotropy ratio $\gamma_{m,cb}=\sqrt{m_c^{¿}/m_b^{¿}}$=15 and $\gamma_{m,cb}=\sqrt{m_c^{¿}/m_b^{¿}}$=9±0.3. If one assumes $\gamma_{m,ca}=\gamma_{m,cb}$ then one obtains $m_{p,ab}$ =3.00673m_e and $m_{p,ab}$=4.22663m_e for the above ratios of Hussey et al., [12] and Taylor et al., [13], respectively. The last two results correspond to the case when $\gamma_{m,ca}=\gamma_{m,cb}$. In reality, there is a slight difference between them: $\gamma_{m,ca}\neq\gamma_{m,cb}$. Kagawa et al., in ref. [14] gives the mass anisotropy ratios for $\gamma_{m,ca}=m_c/m_a$ and $\gamma_{m,cb}=m_c/m_b$ in $YBa_2Cu_4O_8$. So, according to ref. [14] $\gamma_{m,ca}$=13 and $\gamma_{m,cb}$=14. From the latter ratios one obtains

$$\gamma_{m,cab}=\frac{m_c}{m_{ab}}=\frac{m_c}{(m_a\cdot m_b)^{1/2}}=\sqrt{\frac{m_c}{m_a}}\cdot\sqrt{\frac{m_c}{m_b}}=\gamma_{m,ca}\cdot\gamma_{m,cb}=182.$$

Then, using the above mass anisotropy ratio for charge carrier's (polaron's) mass in CuO_2-plane one gets $m_{p,ab}$=3.227m_e . The obtained results are summarised in Table 1. One can notice that the charge carrier's (polaron's) mass in CuO_2-plane is not strongly renormalized as one would expect within ordinary Holstein model. The possibility of existence of light and mobile (bi)polarons in cuprates was pointed out by Alexandrov [15]. From experimental side there are works of Bangura et al., [16] and Yelland et al., [17] reporting on the mass of quasiparticles in $YBa_2Cu_4O_8$ equal to $(2.7\pm0.3)m_e$ and $(3.0\pm0.3)m_e$, respectively. It is seen that our results for the polaron's mass in CuO_2-plane are in good quantitative agreement with the results of experimental measurements on the mass of quasiparticles reported in the works [16,17]. Our findings clearly show relevance of intersite bipolarons and their BEC to cuprates and might overcome existing prejudices with respect to any relevance of (bi)polarons to real oxides.

Table 1

The calculated parameters of $YBa_2Cu_4O_8$ cuprate.

Compound	BEC temperature of the ideal gas of the intersite bipolarons, T_{BEC} (T_c), K	polaron energy, E_p , eV	three-dimensional mass of polaron, m_p , m_e	the mass anisotropy ratio, $\gamma_{m,cab}$	mass of polaron within CuO_2-plane, $m_{p,ab}$, m_e
$YBa_2Cu_4O_8$	80	0.75	18.3	144 [11]	3.489
				225 [12]	3.00673
				81 [13]	4.22663
				182 [14]	3.227

CONCLUSION

In conclusion, we studied $YBa_2Cu_4O_8$ cuprate within the framework of extended Holstein-Hubbard model and bipolaronic mechanism of high-T_c superconductivity. Using analytical formula of BEC temperature of an ideal gas of the intersite bipolarons polaron energy is chosen that provide coincidence T_{BEC} with the experimental value of T_c of $YBa_2Cu_4O_8$ cuprate. Then, having known of E_p we calculated three-dimensional mass of small polaron. Takin experimental values of the mass anisotropy in $YBa_2Cu_4O_8$ cuprate we calculated mass of polaron in CuO_2-plane. Our results show the existence of light (bi)polarons in $YBa_2Cu_4O_8$ cuprate with masses $(3\div4)m_e$ which is compatible with both the experimental value of T_c=80 K and the experimental values of quasiparticle masses reported in the works [16,17].

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